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BIS(2-METHYLMIDAZOLIUM) TETRACHLORODIOXOURANIUM(VI),
 $(\text{CH}_3\text{C}_3\text{N}_2\text{H}_4)_2(\text{UO}_2\text{Cl}_4)^{-2}$

Allan Zalkin, Dale Perry, Leon Tsao,
and Zhang Dechun

January 1983

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BIS(2-METHYLIMIDAZOLIUM) TETRACHLORODIOXOURANIUM(VI),
 $(\text{CH}_3\text{C}_3\text{N}_2\text{H}_4)_2(\text{UO}_2\text{Cl}_4)_2$

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January 1983

ABSTRACT

$M_r = 578.07$, monoclinic, $P2_1/c$, $a = 7.177(2)$, $b = 18.526(4)$, $c = 12.600(3)$ Å, $\beta = 94.08(2)^\circ$, $U = 1671.1$ Å 3 , $Z = 4$, $D_x = 2.30$ g cm $^{-3}$, $\lambda(\text{MoK}\alpha) = 0.71073$ Å, $\mu(\text{MoK}\alpha) = 98.6$ cm $^{-1}$, $T = 23^\circ\text{C}$, $R = 0.035$ for 1501 observed reflections where $F^2 > \sigma(F^2)$.

INTRODUCTION

Uranyl complexes exhibit a highly characteristic luminescence spectrum both in the solution and solid state. This luminescence will often display considerable vibrational structure, and the spectral details are quite dependent on the overall structure of the complex and the nature of the coordination sphere about the central uranyl ion (Brittain and Perry, 1980; Brittain and Perry, 1981; Perry, 1982). The title compound here is being studied in order to better understand its luminescence properties, which are significantly different from those of the unsubstituted imidazolium tetrachlorodioxouranium(VI) complex (Perry, Freyberg, and Zalkin, 1980).

EXPERIMENTAL

The material was made by combining 2-methylimidazole (2 mmole) and uranyl chloride trihydrate (1 mmole) in water, adjusting the pH to 2 with HCl and evaporating to dryness; crystals were obtained by recrystallization from water. A crystal ca. $0.09 \times 0.05 \times 0.20$ mm was mounted with epoxy to a glass fiber and placed on a modified FACS-I Picker diffractometer. About 40 reflections with $20 < 2\theta < 35^\circ$ were used to determine the cell dimensions and their standard deviations. The systematic absences are $h0l$, $l = 2n + 1$ and $0k0$, $k = 2n + 1$. An analytical absorption correction was applied (Templeton and Templeton, 1973) and corrections ranged from 1.52 to 2.68. Intensities were collected to a maximum two-theta value of 45° , and the hkl indices ranged as follows: $-7 \leq h \leq 7$, $0 \leq k \leq 19$, and $-13 \leq l \leq 13$. Three standard reflections ($20\bar{2}$, $\bar{1}\bar{1}\bar{1}$, 040) were measured at every 200th intensity measurement to an accuracy of better than 1.5 percent; the three standards showed isotropic decay of ~25 percent, and the data were adjusted accordingly. A total of 2,740 intensities were measured and resulted in 2183 unique reflections; 550 reflections were measured twice, and the R_{int} from merging these was 0.028. The number of unobserved reflections, $I < \sigma(I)$, was 603. The atomic positions of uranium and chlorine were derived from a three dimensional Patterson function. An electron density map, calculated from the observed structure factors and using phases based on the heavy atoms, revealed the positions of the carbon, nitrogen and oxygen atoms. The F magnitude was used in the full matrix least squares refinement. The calculated non-methyl type hydrogen atomic positional parameters were included in the least-squares calculations but were not refined. Because of

some large discrepancies in the low angle data, all 73 data where $\sin\theta/\lambda < 0.18$ were excluded from the final refinements. The positional and anisotropic thermal parameters for all of the non-hydrogen atoms were included in the refinement. The final weighted R was 0.027 for 1501 data ($F^2 > \sigma(F^2)$), and the goodness of fit was 1.06. The assigned weights, $w = [\sigma(F)]^{-1}$, were derived from $\sigma(F^2) = [C + (pF^2)^2]^{1/2}$, where C is the variance due to counting statistics and p = 0.02.

After the final refinement, the largest shift/error was less than 0.0004. The maximum and minimum heights in the final difference Fourier were 1.23 and -1.20 e/ \AA^3 , respectively. The F(0,0,0) was 1000.5. An empirical extinction correction of the form $F_{\text{corr}} = F_{\text{obs}}(1+kI)$, where $k = 3.5 \times 10^{-6}$, was applied to the data. Scattering factors for U, Cl, O, N, and C were taken from International Tables for X-ray Crystallography (1974). Hydrogen scattering factors used were those of Stewart et al. (1965). Anomalous scattering factors were applied (Cromer and Liberman, 1970), and the f" values used for U, Cl, O, N and C were 9.654, 0.159, 0.006, 0.003 and 0.002, respectively. With the exception of ORTEP, all of the computer programs used in this structure determination were written by the authors for a CDC 7600 computer.

DISCUSSION

The atomic coordinates are given in Table I with the numbering scheme as shown in Fig. 1; a list of distances and angles is given in Table 2.* The structure consists of the packing of columns of $\text{UO}_2\text{Cl}_4^{2-}$ anions and columns of $\text{CH}_3\text{C}_3\text{N}_2\text{H}_4^+$ cations that are parallel to the a axis. Figure 1 shows the view down the a axis of one formula unit.

The $\text{UO}_2\text{Cl}_4^{2-}$ anion is a flattened octahedron with the oxygen atoms occupying the apices and the chlorine atoms the equatorial positions. The anion has been well characterized by other structure determinations, and the distances and angles reported here are in good agreement with those previously determined (Perry, Freyberg and Zalkin, 1980).

The 2-methylimidazolium cation is a planar entity and, with the exception of the methyl group, has the same geometry and dimensions as the unsubstituted imidazolium ion (Perry, Freyberg, Zalkin, 1980). The planes of the two independent 2-methyl imidazolium ions (Fig. 1) are within four degrees of being parallel to each other.

The shortest interatomic distances to the nitrogen atoms are: N(1)-Cl(2), 3.16(1) Å; N(2)-O(1), 3.21(1) Å, N(3)-O(1), 3.12(1) Å; and N(4)-O(2), 3.34(1) Å. These distances are comparable with those in the imidazolium tetrachlorodioxouranium(VI) (Perry, Freyberg and Zalkin, 1980), in which weak hydrogen bonding was suggested.

*Lists of structure factors, anisotropic thermal parameters, and calculated hydrogen positions have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 0000 (11 pp.). Copies may be obtained through the Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

ACKNOWLEDGMENT

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Table 1. Positional parameters and equivalent isotropic thermal parameters (\AA^2).

$$B_{\text{eq}} = \sum_i \sum_j B_{ij} a_i^* a_j^* / 3$$

ATOM	X	Y	Z	B OR BEQ
U	.23303(6)	.12987(2)	.27456(3)	2.82*
CL(1)	-.0723(4)	.12993(16)	.38428(20)	4.10*
CL(2)	.0723(4)	.03771(13)	.13287(21)	3.94*
CL(3)	.5416(4)	.12628(15)	.16763(21)	4.03*
CL(4)	.3920(4)	.22788(14)	.40844(21)	4.15*
O(1)	.1412(11)	.2032(3)	.1970(5)	3.96*
O(2)	.3214(11)	.0564(3)	.3504(6)	4.11*
N(1)	.2030(14)	.8919(5)	.2446(9)	4.08*
N(2)	.2430(14)	.7783(5)	.2461(7)	3.81*
N(3)	.7208(13)	.8607(4)	.2567(6)	3.89*
N(4)	.7125(14)	.9750(4)	.2847(8)	3.49*
C(1)	.2767(17)	.8768(8)	.3438(10)	4.73*
C(2)	.2989(19)	.8036(7)	.3460(11)	4.53*
C(3)	.1836(17)	.8336(7)	.1848(10)	3.51*
C(4)	.1158(21)	.8277(6)	.0711(10)	5.29*
C(5)	.7784(16)	.8711(7)	.3599(9)	3.65*
C(6)	.7767(17)	.9419(7)	.3804(9)	3.96*
C(7)	.6817(16)	.9249(6)	.2111(9)	3.45*
C(8)	.6167(18)	.9370(6)	.0961(9)	4.50*

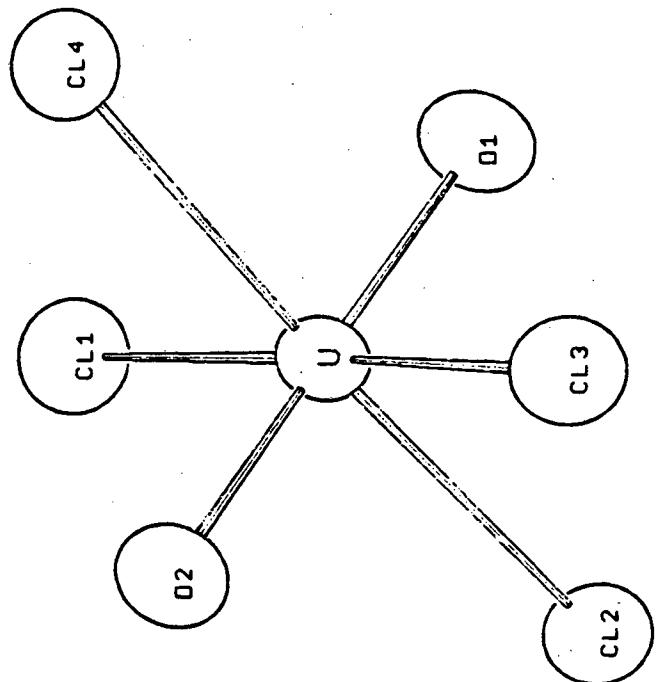
Table 2. Distances (\AA) and Angles ($^\circ$).

U-C1(1)	2.671(3)	N(1)-C(1)	1.35(2)	N(3)-C(5)	1.35(2)
U-C1(2)	2.672(3)	C(1)-C(2)	1.37(2)	C(5)-C(6)	1.34(2)
U-C1(3)	2.674(3)	C(2)-N(2)	1.38(2)	C(6)-N(4)	1.40(3)
U-C1(4)	2.678(3)	N(2)-C(3)	1.33(2)	N(4)-C(7)	1.32(2)
U-O(1)	1.773(6)	C(3)-N(1)	1.32(2)	C(7)-N(3)	1.34(2)
U-O(2)	1.756(7)	C(3)-C(4)	1.48(2)	C(7)-C(8)	1.51(2)

C1(1)-U-C1(2)	90.9(1)	C(3)-N(1)-C(1)	112(1)
C1(1)-U-C1(3)	178.3(1)	N(1)-C(1)-C(2)	105(1)
C1(1)-U-C1(4)	90.1(1)	C(1)-C(2)-N(2)	107(1)
C1(1)-U-O(1)	89.9(3)	C(2)-N(2)-C(3)	109(1)
C1(1)-U-O(2)	89.8(3)	N(2)-C(3)-N(1)	106(1)
C1(2)-U-C1(3)	88.9(1)	N(2)-C(3)-C(4)	125(1)
C1(2)-U-C1(4)	176.9(1)	N(1)-C(3)-C(4)	129(1)
C1(2)-U-O(1)	89.8(3)	C(7)-N(4)-C(6)	109(1)
C1(2)-U-O(2)	89.4(2)	N(4)-C(6)-C(5)	106(1)
C1(3)-U-C1(4)	90.2(1)	C(6)-C(5)-N(3)	109(1)
C1(3)-U-O(1)	91.7(3)	C(5)-N(3)-C(7)	109(1)
C1(3)-U-O(2)	88.6(3)	N(3)-C(7)-N(4)	108(1)
C1(4)-U-O(1)	87.3(2)	N(3)-C(7)-C(8)	126(1)
C1(4)-U-O(2)	93.6(2)	N(4)-C(7)-C(8)	127(1)
O(1)-U-O(2)	179.1(3)		

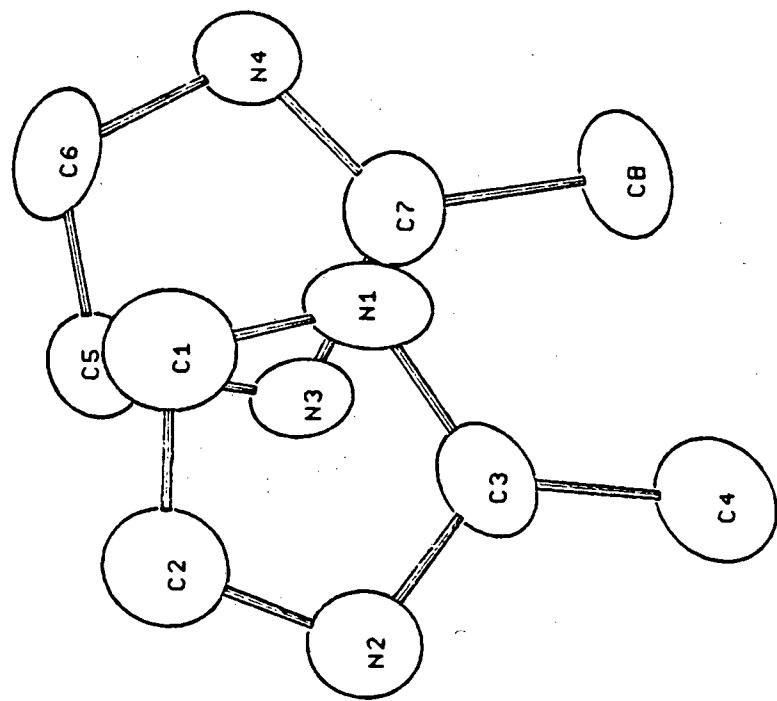
FIGURE CAPTION

Fig. 1. An ORTEP (Johnson, 1965) view of the molecule as viewed down the a axis.



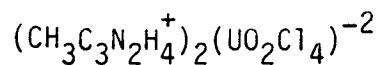
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Fig. 1



SUPPLEMENTARY MATERIALS

BIS(2-METHYLMIDAZOLIUM) TETRACHLORODIOXOURANIUM(VI),



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Anisotropic Thermal Parameters*

ATOM	B11	B22	B33	B12	B13	B23
U	3.521(20)	2.221(17)	2.663(18)	.144(23)	-.187(13)	.197(19)
CL(1)	4.35(14)	4.10(13)	3.88(14)	-.31(15)	.47(12)	-.10(13)
CL(2)	4.94(16)	3.18(12)	3.55(14)	-.56(12)	-.64(13)	-.14(10)
CL(3)	4.17(14)	3.74(12)	4.23(14)	-.25(14)	.62(12)	-.01(12)
CL(4)	5.01(17)	3.81(13)	3.53(14)	-.66(12)	-.38(13)	-.11(11)
O(1)	4.6(4)	3.1(3)	4.0(4)	1.0(3)	-.5(4)	.53(26)
O(2)	4.8(4)	3.4(3)	3.9(4)	.3(3)	-.9(3)	.30(27)
N(1)	4.9(7)	2.5(4)	5.0(7)	.0(4)	.9(5)	.2(4)
N(2)	4.0(5)	3.5(4)	4.0(6)	.6(4)	.8(5)	.2(4)
N(3)	4.4(5)	1.9(4)	2.9(5)	.6(4)	.2(4)	-.0(3)
N(4)	4.4(5)	2.6(4)	3.4(5)	-.3(4)	-.0(4)	-.1(4)
C(1)	4.4(6)	4.4(7)	5.4(8)	-1.0(6)	.2(6)	-.2(6)
C(2)	4.4(7)	4.6(7)	4.4(8)	-1.0(6)	-.2(6)	.1(5)
C(3)	3.3(6)	4.2(6)	3.2(7)	.5(5)	1.1(5)	.8(6)
C(4)	6.8(8)	5.0(6)	4.1(7)	.5(6)	.2(7)	.7(5)
C(5)	4.7(6)	3.4(5)	2.9(5)	-1.0(6)	.3(5)	.2(5)
C(6)	4.4(7)	5.4(7)	2.1(6)	-.6(6)	.4(5)	-.8(5)
C(7)	3.1(6)	4.2(6)	3.1(6)	-1.0(5)	1.0(5)	-.1(5)
C(8)	5.7(8)	5.2(6)	2.5(6)	-.7(6)	-.4(6)	.8(4)

The anisotropic temperature factor has the form $\exp(-0.25(B_{11}h^2a^{}^2 + 2B_{12}hka^*b^* + \dots))$.

Table of Calculated Hydrogen Positions

H(1)	0.1698	0.9372	0.2208
H(2)	0.2419	0.731	0.224
H(3)	0.7072	0.8171	0.2233
H(4)	0.6943	1.0234	0.2739
H(5)	0.3085	0.9111	0.4010
H(6)	0.3473	0.7736	0.4065
H(7)	0.8176	0.8333	0.410
H(8)	0.8126	0.9663	0.4473

OBSERVED STRUCTURE FACTORS, STANDARD DEVIATIONS, AND DIFFERENCES (ALL X 3.0)
 BIS(METHYLLIMIDAZOLIUM)TETRACHLORODICXOURANIUM(VI). F(0,0,0) = 3001

F0B AND FCA ARE THE OBSERVED AND CALCULATED STRUCTURE FACTORS.
 SG = ESTIMATED STANDARD DEVIATION OF FCB. DEL = |F0B| - |FCA|. * INDICATES ZERO WEIGHTED DATA.

L	F0B	SG	DEL	L	F0B	SG	DEL	L	F0B	SG	DEL	L	F0B	SG	DEL		
H, K= 0, 0	2 933	0	0*	H, K= 0, 8	0 815	11	-15	H, K= 0, 12	0 817	10	-2	H, K= 0, 17	8 63	69	-14*		
2 10 24	0 -360*	3 116	0 10*	4 201	0 540	7	5	1 225	5	-9	1 60	64	3*	6 461	6 7	5 191	5 -8
6 8 314	6 3	6 252	5 -3	3 162	4	0	2 663	8 -28	2 566	7 -0	2 72	17 -20	10 0 71	-11*	7 61	58 -11	
12 16	78 -55*	8 188	7 2	5 39	49 22*	4 458	6 -1	4 221	5 11	4 153	8 -1	12 16	78 -55*	8 188	7 2		
H, K= 0, 1	9 131	10 1	6 331	5 -7	7 65	28 -6	6 178	6 1	6 180	8 2	2 295	0 33*	11 77	19 -8			
3 241	0 17*	12 78	36 15	8 169	8 -18	8 199	7 -3	7 79	14 16	7 0	66 -31*	4 61	0 14*	13 38	68 25*		
5 258	5 5	H, K= 0, 5	10 64 -26*	10 0 64 -26*	10 0 76 -51*	1 285	6 3	6 353	5 13	1 109 0 10*	1 13 0 13	2 2180	8 -5	7 335	5 -9	2 183 0 -4*	12 53 75 23*
8 539	7 -5	3 235 4 3	H, K= 0, 9	2 147 6 3	4 132 10 10	9 379	6 5	4 279 4 -4	1 197 4 -1	3 11 61 -13*	5 186 8 6	10 310	6 9	5 226 4 2	2 98 6 -5		
11 250	7 -10	6 309 5 -3	3 148 5 3	5 154 7 -2	1 65 23 13	12 173	9 9	4 192 4 2	6 242 5 -1	2 103 11 19	13 139	12 -16	8 386 6 -5	5 37 37 4*			
H, K= 0, 2	9 289 6 5	6 334 5 -1	8 337 6 -6	4 42 68 33*	0 85	0 5*	10 418 6 -5	7 233 5 -5	9 111 13 2	H, K= 1, 0	1 911	0 54*	11 254 7 6	8 398 6 -12			
2 31	0 21*	12 211 9 -7	9 247 6 4	10 293 7 6 -12	1 210 8 -4	5 228	4 -15	0 100 0 7*	12 135 24 -18	2 194 6 5 -4	0 295	6 143	6 1	1 768 0 38*	H, K= 0, 14 -10		
3 529	0 34*	13 81 56 -12	10 268 7 -12	0 210 8 -4	1 508 6 1 -6	4 149	0 15*	H, K= 0, 6	11 120 13 3	1 543	7 -5	5 228	4 -15	0 100 0 7*	12 135 24 -18		
7 237	5 6	2 157 4 -2	0 329 5 -2	4 160 5 2	2 194 6 5 -4	6 143	6 1	H, K= 0, 10	3 390 5 -13	4 402	0 26*	7 237	5 6	2 157 4 -2	0 329 5 -2		
8 86	26 -9	3 631 7 -20	1 748 9 -4	5 203 6 -3	3 390 5 -13	9 77	16 2	4 124 5 -2	6 105 11 -18	0 117	0 8*	10 62	24 7	5 426 5 -11	3 245 4 1		
11 74	51 -9	6 36 56 2*	4 44 46 15*	8 16 72 -4*	8 16 72 -4*	12 54	72 -25*	7 201 6 -4	5 226 5 -5	9 44 75 -18*	10 278 7 -9	13 70	73 -34*	8 44 57 33*	6 82 20 -0		
H, K= 0, 3	9 19 69 -23*	7 218 6 -11	1 105 8 8	H, K= 1, 1	1 235	0 -13*	10 32 65 8*	8 100 12 0	2 31 60 13*-13	8 292 6 1	2 29	0 -4*	11 50 71 -12*	9 46 60 32*			
3 314	0 16*	12 0 94 -43*	10 63 63 59*	3 212 6 -1	3 314	0 16*	12 0 94 -43*	10 63 63 59*	4 22 64 -31*-11	0 74 -52*	4 308	0 -1*	H, K= 0, 7	11 81 35 13			
5 76	9 -10	1 65 7 4	H, K= 0, 11	5 188 7 2	5 76	9 -10	1 65 7 4	H, K= 0, 11	6 118 10 12 -9	6 62 47 3	6 395	5 2	2 235 4 -6	1 183 5 4			
7 264	5 -6	3 263 4 -5	2 119 6 6	7 180 7 5 -8	7 264	5 -6	3 263 4 -5	2 119 6 6	8 81 19 -20	-7 81 21 6	8 334	6 1	4 145 5 8	1 145 8 -12 -4			
9 448	6 -1	5 389 5 -6	4 4 51 -24*	8 391 7 1 -5	10 287	6 3	6 138 9 -5	5 220 5 7	1 145 8 -12 -4	2 299 8 23*	11 318	6 3	7 406 5 -3	5 220 5 7			
12 157	10 -13	8 324 6 -3	7 387 6 -12	2 327 6 -5	11 318	6 3	7 406 5 -3	6 126 8 8	2 327 6 -5	-3 461 0 20*	13 161	10 -5	9 426 6 -10	8 182 7 -2			
H, K= 0, 4	10 289 6 -11	9 362 6 2	5 118 10 3	5 118 10 3	10 287	6 3	H, K= 0, 4	10 155 9 2	6 122 10 8	1 602 0 1*	0 11 32	0 42*	11 323 7 1	10 155 9 2			
1 84	0 3*	12 154 10 14	11 209 8 3	7 71 33 45	1 84	0 3*	12 154 10 14	11 209 8 3	6 122 10 8	1 602 0 1*	2 586	0 -17*	8 63 69 -14*	8 63 69 -14*			

STRUCTURE FACTORS CONTINUED FOR
BIS(METHYLIIMIDAZOLIUM)TETRACHLORODICOURANIUM(VI).

PAGE 2

L	F08	SG	DEL	L	F08	SG	DEL	L	F08	SG	DEL	L	F08	SG	DEL	L	F08	SG	DEL
3	518	0	12*	3	813	0	-14*	3	729	9	-4	7	143	7	5	H, K=	1,	10	
4	519	6	-12	4	414	5	5	4	714	8	-30	8	28	66	-1*-11	180	10	-10	
5	300	5	-8	5	454	6	0	5	306	4	4	9	65	67	4*-10	78	35	-2	
6	352	5	7	6	275	5	13	6	206	5	2	10	61	61	1*-9	405	6	-3	
7	199	6	2	7	46	65	-12*	7	161	7	4	11	77	28	14	-8	152	9	-20
8	38	59	-34*	8	261	6	6	8	175	7	2	12	84	44	61	-7	507	7	3
9	116	11	-1	9	29	61	6*	9	110	12	-6	H, K=	1,	8	-6	147	7	-3	
10	39	72	21*	10	21	74	-15*	10	101	22	-1	-12	167	10	3	-5	369	5	-1
11	65	22	55	11	44	69	9*	11	51	79	37*	-11	0	71	-58*	-4	67	12	16
12	0	78	-43*	12	117	13	9	12	66	73	28*	-10	251	7	0	-3	245	4	-6
13	69	27	-3	13	68	68	-1*	H, K=	1,	6	-8	466	6	-4	-2	0	53	-22*	
		H, K=	1,		H, K=	1,													
-13	202	9	2	-13	57	68	23*	-11	283	7	3	-6	514	6	-15	0	0	53	-37*
-12	15	52	1*-12	264	7	II	-10	43	72	-2*	-5	206	5	7	1	41	45	94	
-11	228	7	-11	-11	57	65	38*	-9	320	6	-9	-4	354	5	-3	2	42	53	2*
-18	67	38	22	-10	288	6	-5	-8	23	45	8*	-3	33	48	7*	3	210	5	0
-9	452	6	2	-9	84	26	8	-7	556	7	-14	-2	189	4	-1	4	156	6	-4
-8	44	65	36*	-8	489	6	14	-6	121	7	11	-1	124	5	5	5	341	5	-6
-7	682	8	-2	-7	49	60	-12*	-5	677	8	4	0	37	45	26*	6	155	7	-8
-6	73	28	-17	-6	784	9	-4	-4	6	49	-27*	1	89	6	-2	7	333	5	-15
-5	557	7	-1	-5	39	44	29*	-3	291	4	-8	2	160	4	-4	8	65	69	-13*
-4	130	0	18*	-4	570	7	12	-2	174	4	7	3	228	4	-1	9	261	6	-6
-3	362	0	9*	-3	144	0	4*	-1	32	0	3*	4	274	4	-0	10	56	74	1*
-2	191	0	-13*	-2	114	0	-3*	0	207	0	14*	5	255	5	-0	11	294	7	5
-1	268	0	16*	-1	42	0	8*	1	125	4	6	6	319	5	-0	H, K=	1,	11	
0	114	0	-13*	0	130	0	3*	2	99	5	11	7	40	62	-4*-11	56	76	13*	
1	66	0	3*	1	158	0	25*	3	393	5	0	8	290	6	-4	-10	44	72	34*
2	24	0	-13*	2	237	0	8*	4	157	5	-0	9	60	71	17*	-9	43	70	19*
3	375	0	2*	3	225	0	34*	5	342	5	-1	10	304	6	0	-8	48	66	36*
4	209	4	-1	4	522	6	-6	6	29	48	13*	11	108	14	14	-7	163	7	10
5	449	6	-3	5	41	52	14*	7	276	5	4	12	266	8	3	-6	93	12	-4
6	45	51	38*	6	318	5	-1	8	28	68	-13*	H, K=	1,	9	-5	222	6	-5	
7	334	5	-6	7	179	6	4	9	397	6	-1	-12	63	70	16*	-4	173	6	1
8	139	7	5	8	337	6	-4	10	110	13	-5	-11	36	66	-25*	-3	341	5	-0
9	357	6	-3	9	47	67	-12*	11	379	7	9	-10	77	49	40	-2	158	5	-0
10	68	70	12*	10	455	7	-6	12	93	16	47	-9	56	25	16	-1	487	6	4
11	434	7	2	11	40	73	28*	H, K=	1,	7	-8	108	10	1	0	187	5	-1	
12	29	77	9*	12	327	7	9	-12	0	82	-30*	-7	262	5	-2	1	481	6	-5
13	307	8	-0	13	66	49	39	-11	61	78	-6*	-6	218	5	3	2	266	5	-2
		H, K=	1,	3	H, K=	1,	5	-10	63	73	-14*	-5	246	5	-2	3	440	5	-0
-13	89	18	13	-13	78	23	4	-9	44	60	25*	-4	314	5	-1	4	234	5	-1
-12	0	87	-57*-12	70	58	19	-8	56	23	-5	-3	176	5	-2	5	380	5	-1	
-11	128	10	14	-11	56	73	48*	-7	137	7	2	-2	464	6	-1	6	120	9	11
-10	92	27	7	-10	19	64	3*	-6	269	5	-6	-1	313	4	1	7	195	6	-1
-9	37	64	-38*	-9	54	60	22*	-5	364	5	-11	0	615	7	-2	8	43	46	3*
-8	87	13	-5	-8	81	30	0	-4	160	5	-2	1	399	5	-3	9	7	74	-27*
-7	267	5	3	-7	109	3	5	-3	296	4	-6	2	605	7	-8	10	66	39	58
-6	157	6	-3	-6	426	5	5	-2	55	10	-6	3	409	5	-2	11	60	78	38*
-5	461	6	1	-5	350	5	-1	-1	196	4	-4	4	506	6	-5	H, K=	1,	12	
-4	357	5	1	-4	645	7	5	0	211	4	-6	5	342	5	-3	-10	186	8	9
-3	380	0	-2*	-3	261	4	4	1	573	7	0	6	359	5	4	-9	135	10	17
-2	488	0	29*	-2	131	3	-8*	2	436	5	-2	7	115	9	-1	-8	368	6	8
-1	738	0	84*	-1	68	0	10*	3	675	8	-9	8	195	7	-8	-7	115	10	15
0	759	0	81*	0	263	8	-12*	4	417	5	-6	9	51	68	40*	-6	384	5	-11
1	928	0	40*	1	553	0	12*	5	321	5	-3	10	34	71	-20*	-5	92	21	-17
2	715	0	-23*	210	91	0	3*	6	118	7	-5	11	56	77	14*	-4	225	5	-4

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L	F08	SG	DEL	L	F08	SG	DEL	L	F08	SG	DEL	L	F08	SG	DEL				
-3	182	6	-2		H,K=	1,	15	0	46	56	-12*-13	179	14	1	-11	110	19	-2	
-2	133	7	-8	-8	27	87	-14*	1	35	58	-49*-12	0	94	-35*-10	60	81	31*		
-1	79	9	15	-7	90	20	21	2	33	78	12*-11	119	17	4	-9	71	77	17*	
0	91	16	-8	-6	56	38	21	3	92	19	-4	-10	63	85	34*	-8	0	82	-53*
1	104	8	-8	-5	269	8	-6	4	138	13	3	-9	45	56	-5*	-7	154	8	12
2	80	10	4	-4	66	25	-4	5	50	62	-51*	-8	128	13	6	-6	292	6	8
3	38	60	-39*	-3	267	7	1		H,K=	1,	19	-7	0	72	-38*	-5	45	61	18*
4	268	5	-1	-2	78	19	13	-3	166	11	9	-6	89	13	7	-4	567	8	-1
5	65	42	19	-1	188	8	-1	-2	28	82	8*	-5	408	6	8	-3	15	53	6*
6	255	6	-2	0	94	16	0	-1	213	9	10	-4	0	60	-25*	-2	694	9	54
7	91	13	-1	1	425	7	-5	0	66	78	33*	-3	726	10	23	-1	89	0	8*
8	164	8	-3	2	133	11	-6	1	253	9	-0	-2	127	0	5*	0	732	0	54*
9	97	25	7	3	491	6	6	2	79	83	21*	-1	368	0	9*	1	122	5	17
10	228	8	11	4	98	14	9	3	257	9	-1	0	89	0	17*	2	702	9	27
	H,K=	1,	13	5	185	10	0		H,K=	2,	0	1	243	0	13*	3	113	7	1
-10	38	75	15*	6	86	20	9	-12	144	15	-15	2	59	0	15*	4	534	8	-7
-9	49	69	-15*	7	0	85	-71*-10	0	80	-28*	3	559	8	-12	5	73	14	17	
-8	97	26	5	8	86	90	6*	-8	126	14	-10	4	79	13	-2	6	441	7	-13
-7	26	57	12*	H,K=	1,	16	-6	165	9	-11	5	655	9	-29	7	75	19	16	
-6	227	6	-4	-8	213	10	2	-4	734	9	-21	6	92	14	1	8	307	8	-3
-5	97	11	-9	-7	136	13	11	-21450	0	-203*	7	373	7	10	9	0	85	-32*	
-4	269	5	-3	-6	318	8	3	01135	0	140*	8	60	35	13	10	93	22	-8	
-3	197	6	3	-5	150	12	-9	2	356	0	-2*	9	39	85	-40*	11	0	89	-16*
-2	372	5	-3	-4	267	9	1	4	774	10	-62	18	132	13	25	12	23	87	6*
-1	179	5	3	-3	44	75	-15*	6	646	9	-12	11	0	89	-10*	H,K=	2,	5	
0	498	6	-3	-2	111	14	-1	8	216	9	-5	12	0	91	-36*	-12	210	12	-2
1	230	5	1	-1	45	74	2*	10	113	17	-9		H,K=	2,	3	-11	178	11	4
2	489	6	4	0	0	76	-7*	12	34	82	21*-13	192	14	-5	-10	177	11	-3	
3	191	6	-3	1	59	76	-4*		H,K=	2,	1	-12	201	11	3	-9	138	13	-4
4	366	5	-10	2	115	14	-8	-13	158	14	12	-11	259	9	3	-8	286	7	8
5	65	32	-21	3	17	54	-37*	-12	153	15	-7	-10	194	11	6	-7	266	7	4
6	213	6	2	4	182	9	1	-11	240	10	-13	-9	175	11	-6	-6	495	7	3
7	111	10	2	5	93	12	7	-10	287	8	8	-8	234	7	4	-5	375	6	5
8	88	15	-8	6	144	12	-0	-9	241	9	5	-7	223	7	-1	-4	422	6	1
9	72	46	1	7	114	18	29	-8	273	7	12	-6	364	6	5	-3	289	5	-1
10	68	65	26	H,K=	1,	17	-7	218	8	-4	-5	524	8	-4	-2	208	5	-5	
	H,K=	1,	14	-7	79	85	4*	-6	276	6	5	-4	303	5	6	-1	151	5	10
-9	201	8	1	-6	227	9	10	-5	401	6	-6	-3	528	7	17	0	133	6	0
-8	89	27	-26	-5	64	37	-12	-4	539	8	8	-2	189	0	8*	1	15	50	-3*
-7	318	6	3	-4	294	8	-7	-3	658	0	19*	-1	135	0	6*	2	25	52	1*
-6	120	14	-8	-3	28	75	-18*	-2	309	0	11*	0	101	0	-3*	3	128	7	-7
-5	305	6	-5	-2	251	8	-1	-1	575	0	48*	1	72	0	16*	4	199	6	-4
-4	159	7	2	-1	101	15	9	0	87	0	15*	2	206	5	-6	5	154	8	1
-3	95	19	-16	0	334	7	-6	1	40	0	12*	3	76	9	22	6	382	6	5
-2	106	9	-4	1	123	13	-6	2	137	0	22*	4	340	5	1	7	181	9	-5
-1	79	25	-7	2	477	8	-8	3	269	5	23	5	257	6	1	8	388	8	-10
0	40	56	-25*	3	156	11	5	4	226	6	2	6	250	6	13	9	196	9	8
1	61	22	11	4	349	8	-1	5	202	7	-17	7	411	7	2	10	251	9	14
2	106	12	19	5	109	17	-12	6	537	8	-1	8	218	9	11	11	131	15	17
3	186	8	-7	6	146	14	-4	7	214	7	17	9	235	9	-13	12	128	17	5
4	77	17	27	H,K=	1,	18	8	290	7	6	10	184	11	1	H,K=	2,	6		
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6	118	13	-2	-4	0	86	-68*	10	167	12	-5	12	159	14	-2	-11	157	12	14
7	120	14	-5	-3	168	11	-6	11	243	10	-14		H,K=	2,	4	-10	0	83	-32*
8	157	12	13	-2	0	73	-13*	12	242	10	5	-13	0	96	-67*	-9	0	80	-27*
9	245	9	13	-1	0	87	-45*	H,K=	2,	2	-12	140	16	5	-8	51	83	-40*	

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L	F08	SG	DEL	L	F08	SG	DEL	L	F08	SG	DEL	L	F08	SG	DEL	L	F08	SG	DEL
-10	71	87	11*	-6	118	11	-4	0	813	11	35	8	190	9	13	-5	289	6	10
-9	113	15	5	-5	38	69	-33*	1	538	7	-7	9	108	16	28	-4	97	13	7
-8	45	55	4*	-4	226	6	0	2	538	8	13	10	106	20	7	-3	371	6	7
-7	0	79	-13*	-3	420	6	3	3	243	6	-2	11	0	91	-8*	-2	79	14	13
-6	57	70	19*	-2	446	7	-5	4	240	6	3	H, K=	3,	8	-1	260	6	3	
-5	219	6	6	-1	753	10	38	5	250	6	6	-11	83	29	9	0	0	65	-26*
-4	232	6	2	0	632	8	11	6	387	7	6	-10	335	9	-1	1	101	11	1
-3	407	6	1	1	549	7	1	7	275	8	-1	-9	122	15	-3	2	62	20	0
-2	486	7	6	2	379	5	-2	8	305	8	3	-8	371	7	-1	3	0	68	-43*
-1	457	6	10	3	324	5	-2	9	115	14	14	-7	130	10	16	4	16	73	-29*
0	450	6	12	4	259	6	3	10	72	86	2*	-6	262	7	1	5	187	0	-1
1	381	6	2	5	223	7	-1	H, K=	3,	6	-5	90	12	13	6	0	52	-48*	
2	362	5	-3	6	349	7	4	-12	0	86	-24*	-4	277	6	-2	7	249	8	-4
3	312	6	-7	7	258	8	-1	-11	260	10	12	-3	184	7	-15	8	60	81	-21*
4	363	6	1	8	213	9	-1	-10	62	34	45	-2	318	6	5	9	290	9	2
5	286	6	10	9	228	9	11	-9	401	8	2	-1	156	7	-2	10	124	17	19
6	263	7	10	10	19	85	-20*	-8	78	21	18	0	227	5	6	H, K=	3,	11	
7	222	8	11	11	0	88	-40*	-7	436	7	6	1	126	8	-5	-10	75	86	3*
8	175	11	-3	H, K=	3,	4	-6	0	72	-20*	2	97	10	10	-9	58	84	9*	
9	108	19	-17	-12	192	13	6	-5	263	6	3	3	115	9	-1	-8	21	55	-13*
10	135	14	18	-11	76	82	43*	-4	68	14	14	4	110	10	10	-7	0	74	-21*
11	30	91	-36*	-10	334	3	4	-3	230	6	1	5	62	24	-11	-6	74	20	19
12	53	91	50*	-9	89	20	12	-2	133	7	-3	6	249	7	2	-5	151	9	0
H, K=	3,	2	-8	487	8	6	-1	309	5	13	7	36	74	22*	-4	115	12	4	
-12	54	86	38*	-7	39	77	-36*	0	118	7	10	8	297	8	-2	-3	344	7	0
-11	319	9	-1	-6	380	6	-6	1	123	8	-4	9	128	14	8	-2	141	9	-0
-10	0	89	-11*	-5	96	11	-5	2	127	8	1	10	247	10	-6	-1	392	6	4
-9	454	8	0	-4	276	5	4	3	0	65	-33*	H, K=	3,	9	0	188	7	14	
-8	0	78	-6*	-3	20	55	7*	4	61	63	36*	-11	71	87	27*	1	360	6	1
-7	332	8	-13	-2	453	7	1	5	177	7	5	-10	134	14	33	2	185	7	1
-6	52	33	-5	-1	62	12	-4	6	44	50	27*	-9	85	21	7	3	400	7	16
-5	362	6	9	0	339	5	3	7	357	7	-4	-8	0	83	-35*	4	152	9	1
-4	104	9	10	1	204	5	3	8	112	16	-19	-7	0	76	-54*	5	296	7	-9
-3	564	8	8	2	41	56	29*	9	334	8	15	-6	76	17	14	6	126	12	10
-2	33	52	22*	3	53	64	-22*	10	46	88	-26*	-5	56	71	17*	7	160	11	-3
-1	428	6	13	4	89	12	-1	11	183	13	-4	-4	231	6	3	8	106	16	23
0	102	7	-1	5	201	7	-13	H, K=	3,	7	-3	236	6	-2	9	109	19	1	
1	83	8	6	6	274	7	-3	-11	156	13	20	-2	446	6	0	H, K=	3,	12	
2	198	5	5	7	115	13	25	-10	28	59	-14*	-1	354	6	3	-9	0	94	-96*
3	0	63	-70*	8	452	7	3	-9	24	82	-55*	0	523	8	9	-8	250	8	2
4	0	66	-41*	9	44	82	4*	-8	21	79	-27*	1	279	6	4	-7	79	80	-5*
5	141	10	-14	10	312	9	11	-7	65	77	-6*	2	473	7	4	-6	211	8	4
6	161	9	6	11	0	62	-11*	-6	0	74	-23*	3	237	6	8	-5	152	9	1
7	345	7	8	H, K=	3,	5	-5	124	10	0	4	417	7	-0	-4	291	7	-1	
8	0	80	-33*	-12	104	20	19	-4	17	63	-44*	5	178	8	7	-3	142	9	1
9	448	8	-3	-11	86	24	13	-3	210	6	3	6	320	7	-6	-2	316	6	2
10	32	85	23*	-10	99	18	34	-2	342	5	6	7	116	14	-8	-1	0	71	-28*
11	333	9	12	-9	63	34	-19	-1	508	7	5	8	204	10	-2	0	145	9	5
12	56	60	24*	-8	65	27	25	0	378	5	4	9	86	92	-41*	1	66	67	56*
H, K=	3,	3	-7	27	72	15*	1	535	7	-3	10	48	93	-43*	2	0	72	-23*	
-12	0	92	-59*	-6	173	8	9	2	239	5	-4	H, K=	3,	10	3	40	70	27*	
-11	134	17	-14	-5	75	14	6	3	283	6	-4	-10	100	21	10	4	78	18	8
-10	66	89	-27*	-4	132	8	1	4	135	8	3	-9	319	9	-10	5	0	78	-46*
-9	36	82	29*	-3	110	8	-1	5	251	7	-5	-8	54	80	-10*	6	103	16	-19
-8	62	30	27	-2	357	5	-1	6	118	13	-6	-7	233	8	8	7	28	86	-35*
-7	94	13	25	-1	448	6	3	7	255	8	4	-6	40	73	-9*	8	238	9	2

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L	F08	SG	DEL	L	F08	SG	DEL	L	F08	SG	DEL	L	F08	SG	DEL				
9	65	83	-11*	-2	164	10	1	5	61	78	10*	-10	58	89	-24*	1	570	8	2
H, K=	3,	13	-1	170	9	12		6	150	12	-1	-9	48	85	2*	2	98	11	2
-9	0	94	-54*	0	100	17	-5	7	135	12	10	-8	62	80	45*	3	510	7	1
-8	0	84	-37*	1	0	83	-71*	8	142	14	0	-7	56	75	34*	4	61	72	-13*
-7	28	55	3*	2	48	79	28*	9	269	9	9	-5	19	68	2*	5	407	7	-2
-6	74	78	4*	3	0	77	-18*	10	253	10	6	-4	151	8	1	6	81	19	2
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-3	105	14	-5	H, K=	3,	17	-12	0	94	-3*	-1	41	59	27*	9	134	15	14	
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2	303	6	-1	-1	136	13	-0	-7	0	55	-23*	4	403	7	-8	-9	262	9	-1
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6	210	9	-1	3	98	17	17	-3	121	9	1	8	213	10	5	-5	269	7	2
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8	204	10	13	H, K=	3,	18	-1	216	6	-1	10	89	26	-14	-3	225	6	1	
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2	0	74	-38*	-6	76	85	-49*	11	90	28	3	-2	253	5	3	8	0	86	-69*
3	67	23	18	-4	387	7	10	H, K=	4,	3	-1	160	7	-6	9	163	13	-6	
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2	51	32	-32*	-5	425	7	3	3	60	66	-4*	-9	71	86	-5*	2	618	9	12
3	172	10	-2	-4	257	7	1	4	0	72	-39*	-8	41	54	11*	3	119	11	-3
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-5	124	13	23	2	80	15	-7	10	157	15	-11	-2	46	31	13	9	45	58	32*
-4	172	10	5	3	60	23	4	H, K=	4,	4	-1	441	6	8	H, K=	4,	9		
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L	F08	SG	DEL	L	F08	SG	DEL	L	F08	SG	DEL	L	F08	SG	DEL
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-6	322	7	3	-6	65	81	-22*	3	39	79	2*	-1	187	7	-9
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1	188	7	10	1	140	9	12	0	243	9	-0	6	16	80	-10*
2	0	73	-41*	2	452	7	3	1	137	11	18	7	196	11	-3
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7	49	76	22*	7	0	79	-59*	0	136	13	9	-9	69	82	19*
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	H,K=	4,	10	-3	248	18	6	-10	82	91	-1*	-7	51	76	6*
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6	63	27	14	-3	166	10	-4	-7	294	8	-2	7	7	60	-44*
7	76	82	-17*	-2	69	74	23*	-6	40	74	13*	8	143	14	3
8	105	18	5	-1	162	11	9	-5	464	7	-13	9	0	85	-6*

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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
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H,K=	5,	8	-5	110	15	6	-2	228	7	-8	6	86	92	-15*	-4	107	15	-19	
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-8	165	12	-2	-3	130	12	-19	2	225	8	6	H,K=	6,	4	-2	186	9	-8	
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-5	124	12	-2	0	94	15	14	H,K=	6,	1	-6	0	82	-14*	1	115	13	-6	
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-2	264	7	-10	3	297	7	4	-7	86100	-74*	-3	0	74	-44*	4	0	81	-5*	
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4	0	54	-59*	-6	289	8	6	-1	193	8	-9	3	43	76	-7*	-5	0	78	-21*
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6	94	19	-11	-4	300	3	3	1	146	10	5	5	0	81	-24*	-3	61	75	0*
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8	123	16	3	-2	167	10	6	3	39	80	-48*	7	36	84	18*	-1	105	14	-4
H,K=	5,	9	-1	94	14	30	4	0	57	-28*	H,K=	6,	5	0	260	6	-13		
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-7	29	77	13*	1	0	80	-42*	6	0	97	-54*	-7	61	40	-12	2	229	6	-9
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-5	83	19	-3	3	0	78	-3*	H,K=	6,	2	-5	131	12	0	4	205	9	6	
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-3	111	13	1	5	50	77	34*	-7	0	84	-28*	-3	210	8	-6	H,K=	6,	9	
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0	245	7	-8	-5	0	82	-6*	-4	74	20	18	0	105	14	-25	-4	162	10	2
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2	315	7	-9	-3	58	72	34*	-2	0	72	-29*	2	56	69	6*	-2	195	6	5
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4	310	7	-4	-1	43	79	-31*	0	0	73	-17*	4	47	53	36*	0	161	10	-2
5	163	10	-1	0	153	11	-4	1	289	7	-1	5	58	79	50*	1	0	77	-54*
6	237	9	-5	1	0	82	-61*	2	0	76	-58*	6	76	81	10*	2	84	19	5
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-8	0	59	-33*	4	244	9	4	5	256	9	-9	-8	0	86	-4*	5	13	82	-30*
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-5	351	7	4	-3	259	8	16	H,K=	6,	3	-5	78	19	29	-4	0	80	-20*	
-4	54	77	-10*	-2	0	82	-58*	-9	143	16	2	-4	19	73	15*	-3	62	75	-13*
-3	260	7	-0	-1	45	88	-71*	-8	124	17	11	-3	159	10	-10	-2	0	80	-63*
-2	0	72	-14*	0	24	80	-32*	-7	137	14	-1	-2	67	70	12*	-1	188	9	5
-1	172	8	1	1	63	75	18*	-6	60	82	-36*	-1	237	5	-2	0	119	12	27
0	0	74	-24*	2	0	81	-22*	-5	166	11	-12	0	50	72	2*	1	211	9	-10
1	122	12	-4	3	74	84	29*	-4	111	15	-14	1	223	5	-4	2	78	81	19*
2	39	51	-18*	H,K=	5,	15	-3	285	7	5	2	59	73	18*	3	77	86	-46*	
3	0	52	-8*	-2	0	83	-55*	-2	124	12	-1	3	256	8	-2	4	0	81	-36*
4	65	26	59	-1	156	12	-6	-1	232	8	-6	4	50	80	-15*	H,K=	6,	11	
5	46	84	-42*	0	70	79	19*	0	130	10	6	5	257	9	-6	-4	32	83	-51*
6	100	16	29	1	116	16	-6	1	64	70	3*	6	0	90	-48*	-3	172	10	3

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